Chapter 8
Mathematical Simulation of Blast Furnace Operation

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Abstract This chapter deals with possibilities of mathematical modeling of blast furnace operation. This chapter summarizes various attitudes for evaluation of blast furnace operation. The chapter is aimed at modeling of kinetics of reduction processes. It presents a methodology developed at VŠB—Technical University of Ostrava—for interpreting of laboratory tests carried out according to international standards such as ISO 4695:2007. The designed model uses laboratory test results as inputs for mathematical simulation of the material processing in blast furnace aggregate. The model calculates kinetic constants of changes in iron oxides concentration during nondirect reduction and estimates coke consumption for it. It presents simulation of reduction gas consumption regarding the ratio of direct reduction in time. It carries out simulation for one-component and two-component blast furnace feedstock to find easily the optimum of production process.

8.1 Introduction

Centre ENET goes on with the development of mathematical model using Rist's diagram and former knowledge for simulation of reduction process in blast furnace (Bilík 1990). Reduction model was developed in three stages (from Fe_3O_4 to Fe_2O_3, then to FeO, and finally to Fe). In equations, it was required to use kinetic constants of single chemical reactions. Edge and initial conditions of partial differential equations were determined by two exercises (Pustejovska et al. 2013, 2015).

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The first exercise was reduction on rigid bed with a great surplus of reduction gas, which is enabled by experimental laboratory equipment. Solution of equations is analytic, in the form of formula where there was amount of sample mass loss on the left side and on the right side there was a complicated expression depending on the sample initial composition and kinetic constants, which cannot be found in any textbook or technical literature. Experimental data (sample mass loss in time) are possible to use to reveal a theoretic function such values of kinetic constants for which theoretic time flow and time of mass loss measured during the test is almost the same. These quasi(kinetic) constants of ore gas reduction gained from experimental data are fundamentally new partial result of the methodology.

The second exercise was reduction simulation in countercurrent in the blast furnace stack. The information about chemical composition and kinetic constants of chemical reactions found out from the first exercise are input data using for the calculation. Calculation result is "practically reachable" coke minimum specific consumption (ω). Classical heat balance needs reducing gas composition on the furnace top to check coke-specific consumption at blast furnace. To calculate "theoretic minimum" coke consumption, it is necessary to assume reaching chemical equilibrium between gas and charge, which can originate only after infinite time of charge holding at blast furnace. Presented use of kinetic constants enables calculation of coke consumption for actual charge under current conditions of present blast furnace (Jursová and Bilík 2013).

8.2 Kinetic Model of Reduction

8.2.1 Simulation of Reduction in the Fixed Bed

The laboratory tests of the blast furnace burden reducibility are carried out in a stationary fixed bed. The height of the burden bed is made small, and at the same time, the amount of reduction gas is large. Consequently, the change of the molar O/Fe ratio in the burden and the molar O/C ratio in the gas along the coordinate of the fixed bed is small, and the derivatives with respect to the coordinate can be dropped.

$$\frac{\partial C_i}{\partial t} = -K_i C_i \left(X - X_{e,i}\right) + K_{i-1} C_{i-1} \left(X - X_{e,i-1}\right) \tag{8.1}$$

where C_i is Fe concentration in the ith form as the fraction of the entire amount of Fe in the charge, K_i is kinetic constant (s^{-1}), X is molar O/Fe ratio in the burden, and $X_{e,i}$ is equilibrium molar fraction of CO with Fe in the ith form. The model yields a system of ordinary linear differential equations with initial determined by the values of the concentrations of Fe in the form i. The model can be solved analytically yielding the following result:

$$C_1\left(t\right) = C_{1,0} e^{-N_1 t} \tag{8.2}$$

$$C_2\left(t\right) = C_{2,0} - \frac{C_{1,0}N_1}{N_2 - N_1}e^{-N_2 t} + \frac{C_{1,0}N_1}{N_2 - N_1}e^{-N_1 t} \tag{8.3}$$

$$\begin{aligned} C_3\left(t\right) = C_{3,0} - \frac{C_{2,0} - N_2}{N_3 - N_2} + \frac{C_{1,0}N_1N_2}{\left(N_3 - N_1\right)\left(N_3 - N_2\right)}e^{-N_3 t} + \frac{C_{2,0-}N_2}{N_3 - N_2} \\ + \frac{C_{1,0}N_1N_2}{\left(N_3 - N_1\right)\left(N_3 - N_2\right)}e^{N_2 t} + \frac{C_{1,0}N_1N_2}{\left(N_3 - N_1\right)\left(N_3 - N_2\right)}e^{-N_1 t}. \end{aligned} \tag{8.4}$$

where $C_{i,0} = C_i(0)$ is the initial concentration of Fe in the form $i = 1, 2, 3$ for $t = 0$, and N_i expressed (8.5).

$$N_i = K_i\left(X_0 - X_{e,i}\right), \quad i = 1,2,3 \tag{8.5}$$

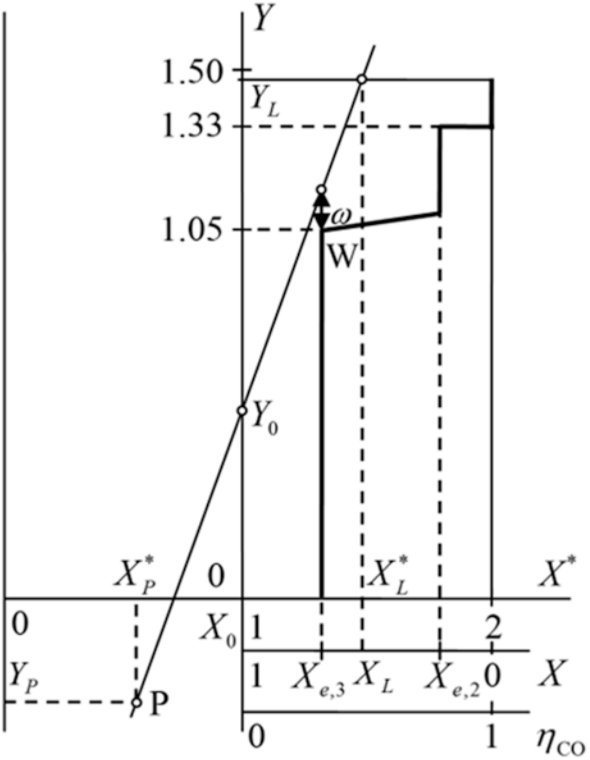
The composition of the reduced burden is given by its content of Fe_2O_3 and FeO. In calculating the initial values of the concentration C_i, it is assumed that the sample does not contain elementary iron ($C_4 = 0$) and that iron is combined only in the form of Fe_3O_4 ($C_3 = 0$). *e* equilibrium constants were taken from the literature. The weighted sum of the concentrations C_1, C_2, and C_3 gives the molar O/Fe ratio in the sample of the burden. Of course, in order to calculate the time dependence $Y_{(t)}$ in the analytical form, it is necessary to determine the kinetic constants K_1, K_2, and K_3. These can be determined using the least squares method from the experimentally recorded time history of the mass loss of the oxygen in the sample during reduction and fitting them to the mass loss calculated from the analytical form of $Y_{(t)}$. The difference between calculated $Y_{(t)}$ and the experimental value Y_j forms the objective function (8.6)

$$F\left(K_{1,}K_{2,}K_3\right) = \sum_j \left(Y_j - Y_{\left(t_j\right)}\right)^2. \tag{8.6}$$

The objective function depends nonlinearly on the sought parameters, and it is therefore difficult to determine the global minimum. The optimization was therefore repeated for various initial estimation of the parameters K_1, K_2, and K_3 to locate global minimum. The kinetic constants for the given temperature of reduction characterize the reducibility in greater detail in comparison with the characteristics such as the amount of oxygen reduced in 1 h. To calculate the kinetic constants, it is necessary to have data describing the chemical equilibrium between the oxides of iron and between the composition of the reducing gas and the burden (Mihok and Baricová 2008).

Model simulation of reduction in countercurrent flow results from Rist's diagram. The slope of operating line in Rist's diagram (Fig. 8.1) represents the specific consumption of the reduction gas determined by the number of kmoles of CO per kg of Fe in the countercurrent phases (Konstanciak et al. 2003). Calculation of the

Fig. 8.1 Rist's diagram for iron ore reduction



position of the operating line is repeated for several values of the specific consumption of the reduction gas CS. This yields a set of operating lines whose positions are expressed by approximation Eq. (8.7). The parameter has been used for evaluation of the reducibility of the burden in the blast furnace by calculating this parameter from the O/Fe of the burden reduced in the direct way (r_d) and the composition of the burden, the gas at the top of the reduction zone (X_L, Y_L). The value of parameter determined from the laboratory tests of the ore reducibility can be compared with the value of the parameter determined from the operating data of the blast furnace. Better reducibility of the ore burden is characterized by the low value of the parameter ω.

$$\omega = a_0 + a_1 CS + a_2 CS^2. \tag{8.7}$$

8.2.2 Calculation of Specific Carbon Consumption

The specific consumption of the reducing gas is identical with the specific consumption of the carbon required to produce this gas (Babich et al. 2008). For the modeling, the calculation is carried out by Rist's diagram. Therefore, the set of the operating straight lines for the given ore burden specifies the relationship between the specific consumption of the reducing gas and the degree of the direct reduction depending on the value of the parameter ω. The holding reaction time can be determined from a blast furnace production rate and volume. The production rate results also for the intensity of heat transfer in the lower and upper zone of the blast furnace. The heat balance equation of the lower zone for 1 kg of it is as follows:

$$\left(CS-Y_f-Y_0\right)q_v=Y_0q_d+Q. \tag{8.8}$$

The quantity Y_f designates the consumption of carbon for reduction of accompanying elements. The left-hand side represents the heat released by imperfect combustion of carbon in front of the tuyeres and the sensible heat of the hot blast transferred to the burden by cooling to the temperature of the thermally ineffective zone. The first term on the right-hand side of Eq. (8.8) is the consumption of the heat for direct reduction, and the second term is the heat for reduction of accompanying elements, melting and heating the products of the melt to the tapping temperature and to cover heat losses. The thermal balance equation makes/enables us to write the equation of the operating line in the following form (8.9):

$$Y=Y_0\left(X^*-\frac{q_d}{q_d+q_v}\right)\frac{q_v}{q_d+q_v}+\left(Y_f+\frac{Q}{q_d}\right)\left(X^*-1\right) \tag{8.9}$$

This form of equation of the operating line indicates that the position of its point P has the coordinates

$$X_p^*=\frac{q_d}{q_d+q_v},Y_p=\left(Y_f+\frac{Q}{q_d}\right)X_p^*-Y_f. \tag{8.10}$$

As it is shown in Fig. 8.7, the position of the point P is determined by parameters controlled by composition of the burden and hot metal, blast temperature, the temperature of the isothermal zone, and slag and the heat losses. This indicates that the main problem of calculating the specific consumption of carbon is the construction of the operating line which passes through the point P and is also included in the set of the straight lines for the specific burden. The calculation results in the theoretically minimum consumption of carbon for production of hot metal which is discussed in literature as the ideal blast furnace operation in case that operating line passes through the point W, the calculation results in the theoretically minimum consumption of carbon for production of hot metal which is discussed in literature as the ideal blast furnace operation. The positive value of the parameter ω introduces into the calculation of the specific consumption CS the dependence on the reducibility of the ore burden. The result of calculation may be considered as the prediction of the consumption of carbon for a given ore burden in the blast. The calculation procedures also take into account the presence of hydrogen in the reduction gas and decomposition of carbonates.

8.3 Practical Modeling of Results of Reducibility Test

Parameters of measurement are indicated in Table 8.1. The Levenberg-Marquardt method was used for optimization of function $F(k_1,k_2,k_3)=\Sigma(Y_j-Y(t_j))^2$. Optimization was programmed using MATLAB mathematical library. Calculated kinetic constants are an important starting parameter during simulation of reduction processes of iron oxides in the stack of blast furnace. Calcualted kinetic constants are an important starting parameter during simulation of reduction processes of iron oxides in the stack of blast furnace (Bilík and Vu 2000). For practical modeling were used the samples of the properties presented in Table 8.2.

8.3.1 Example of Calculation of Reduction Run in the Area of Indirect Reduction

Results of reducibility test were used for simulation of different model options of indirect reduction of iron oxides (Pustějovská and Jursová 2013a, b). Proportion of direct/indirect reduction ideally represents proportion of wüstite in reduced charge when area-relative height of indirect reduction is zero. Below it, Boudouard's reaction already starts.

Figures 8.2 and 8.3 present reduction run of sinter of grain size amounting to 10–12.5 mm with time period of charge keeping in reaction space of duration of 3 h and with reducing gas-specific consumption amounting to 2 kmol^{-1} of Fe.

Figure 8.4 presents reduction of two-component charge with different compositions: Two sinters were selected (sinter 1, 10–12.5 mm, and sinter 2, 10–12.5 mm). Dependence of controlled quantities (composition of reducing gas, concentration of iron oxides) is graphically represented. This calculation can serve in providing optimum charge composition for given technological conditions.

Mutual dependence among carbon consumption, direct reduction level, and process intensity following kinetic model application has generally tridimensional form. It is obvious that the lowest coke consumption is in the optimal rate between

Table 8.1 Parameters of reducibility tests

Sample weight	500 g
Measurement temperature	950 °C
Reducing gas composition	40 % CO, 60 % N_2
Gas equilibrium concentrations	$X_{r1}=0.01$; $X_{r2}=0.198$; $X_{r3}=0.675$

Table 8.2 Properties of samples

Sample	Fe [%]	FeO [%]	P_2	dR/dt
1	54.9	7.33	1.07	1.01
2	56.00	10.9	1.1	0.52

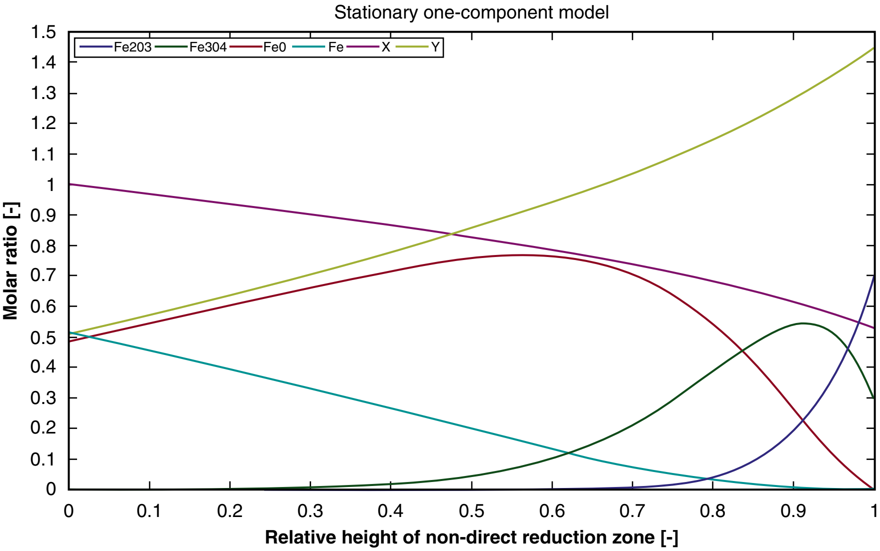


Fig. 8.2 Gas oxidation grade during decline of sinter 1 in the area of indirect reduction at the stack

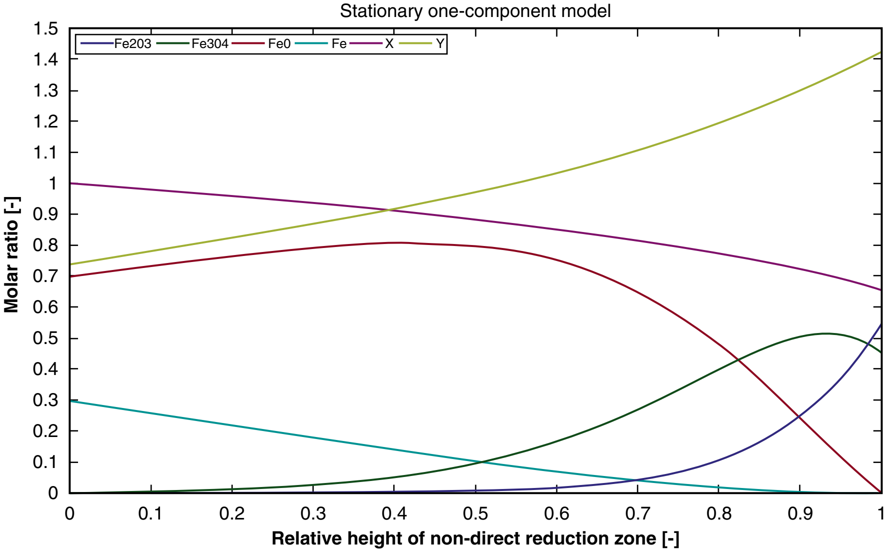


Fig. 8.3 Gas oxidation grade during decline of sinter 2 in the area of indirect reduction at the stack

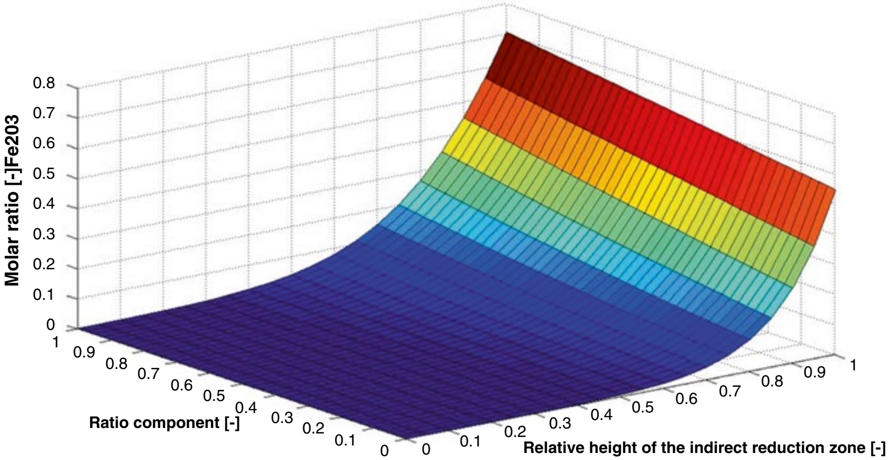


Fig. 8.4 Dependence of magnetite concentration on sinter relative height and its share in feedstock

direct and nondirect reduction. A different ratio results in an increase of coke consumption. The model interpretation has to respect the real dynamics of blast furnace technology. The productivity of blast furnace aggregate is affected by feedstock descent. The rate affects on the time of feedstock stay in the area of nondirect reduction. The shorter time results in the increase in ratio of direct reduction and the increase of heat demand relating to coke consumption (Jursová et al. 2015). An optimizing area for the specific consumption of reduction gas, relating to the time of stay in nondirect reduction area and direct reduction rate, is depicted Fig. 8.5. In case of usage of sinter 1, the optimizing area for the specific consumption of reduction relating to the time is typical with lower ratio of direct reduction, and for optimized blast furnace, feedstock processing in the zone of nondirect reduction rate is required shorter time. The comparison is obvious from Fig. 8.6.

Figures 8.6 and 8.7 present the time effect of feedstock stay in the area of nondirect reduction. It presents the changes in limit kinetic curves of carbon consumption at time of feedstock stay in the area of nondirect reduction. As the time is shorter, the limit kinetic curve of carbon consumption is of higher values.

8.3.2 *Use of Kinetics Simulation for CDR Diagram Modification*

By gaining kinetically well-founded dependence between reducing gas-specific consumption and level of direct reduction, it can be then determined chemical-kinetic limit of carbon consumption on indirect reduction of iron oxides expressed by the curve showed on Fig. 8.8. From the point of view of enthalpy balance, it is also necessary to provide that heat developed during carbon gasification to reducing gas will

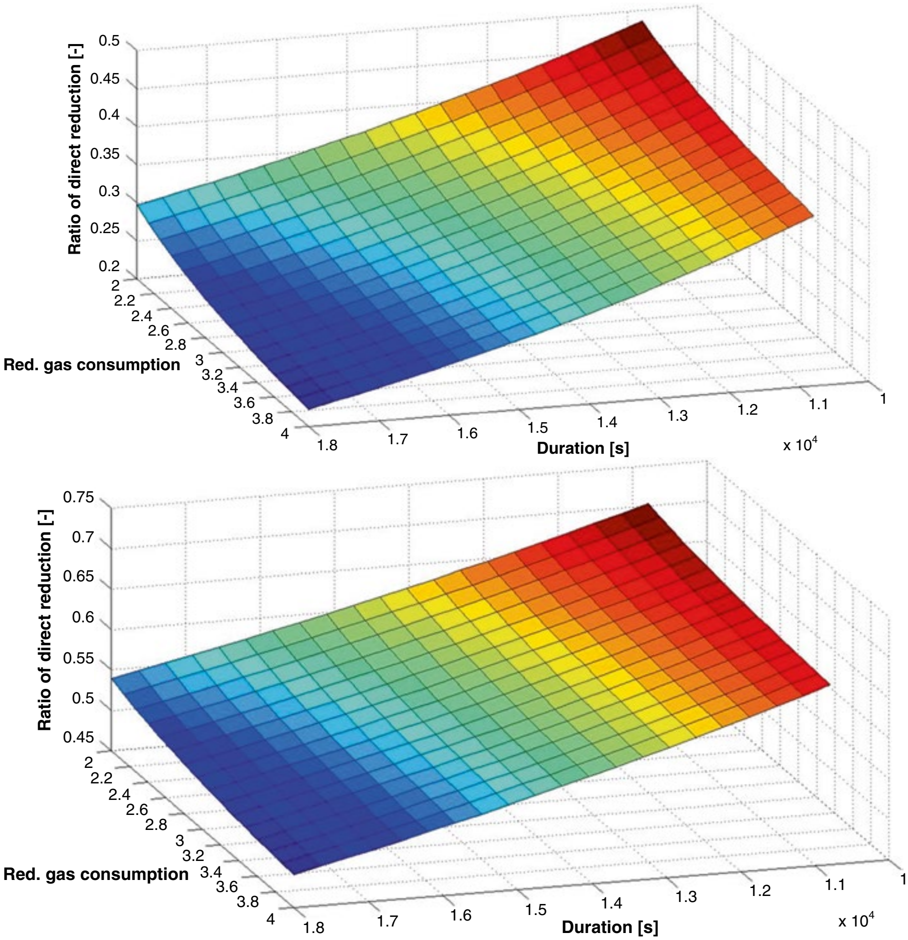


Fig. 8.5 (**a**) Optimizing possibilities for sinter 1; (**b**) Optimizing possibilities for sinter 2

cover also necessary heat needs of the process. Carbon needed for heat (heat limit) also depends significantly on the level of direct reduction. As indirect reduction is applied in the first phase of blast-furnace smelting, its run extent is in principle decisive for resulting mutual ratio of both reduction types (Jursová et al. 2013). Therefore the key role falls on kinetic simulation of indirect reduction run of iron oxides. Output of this simulation is a share of direct reduction on complete reduction extent—level of direct reduction rd. Mutual dependence between direct reduction share and resulting consumption of fuel carbon/deoxidizing agent represents a requirement on real minimum provision of reduction process by this fuel/deoxidizing agent.

In Fig. 8.9, there are kinetic curves as well as intersection of these curves with heat limit (point) calculated for conditions of present Czech process conditions. In comparison with currently used CDR diagram form, version mentioned in Fig. 8.8

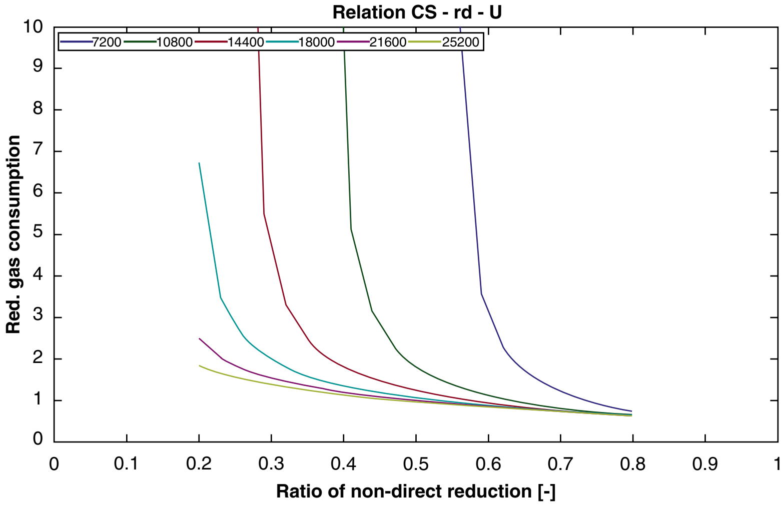


Fig. 8.6 Carbon consumption for processing of sinter 1 at nondirect reduction

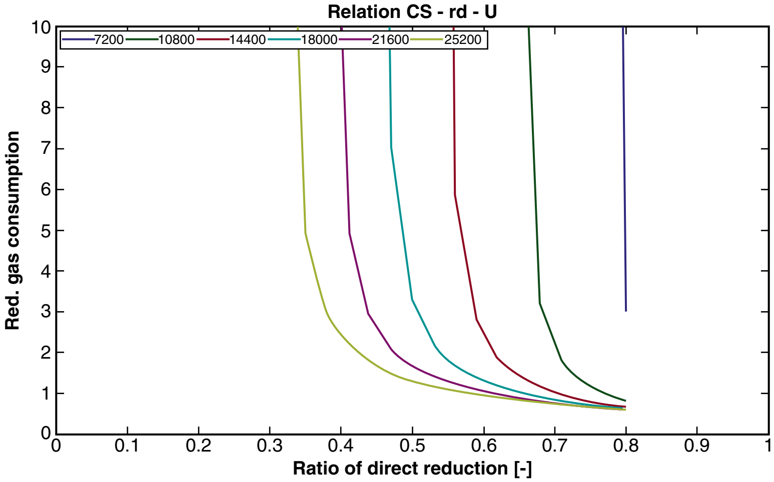


Fig. 8.7 Carbon consumption for processing of sinter 2 at nondirect reduction

shows not only theoretic but rather real limits of minimum specific consumption of reducing gas respecting actual charge reducibility and which can be reached only through better use of reducing gas (Bilík et al. 2013).

Mathematic model based on the indirect reduction describes well the reduction course in the area of the blast furnace where speed of Boudouard's reaction is small. But this model can also be successfully applied at simulation of reduction process of the so-called direct iron production where coke is not used or for estimation of proportion of direct/indirect reduction during processes of melting reduction.

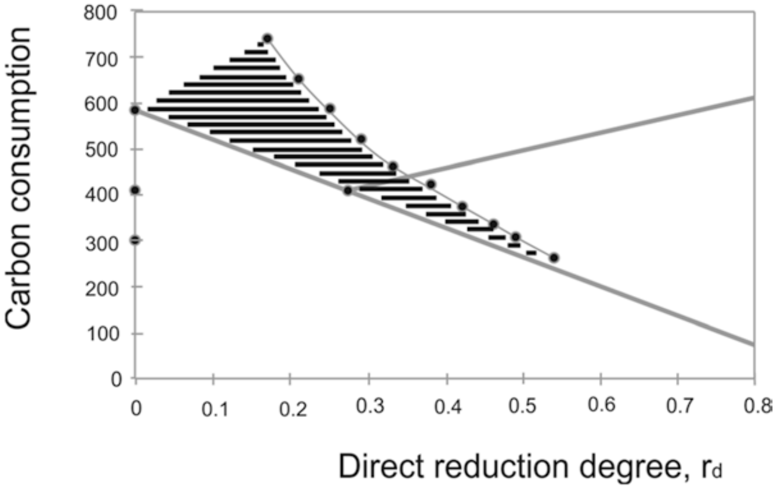


Fig. 8.8 Dependence of reducing gas (carbon)-specific consumption on the level of direct reduction

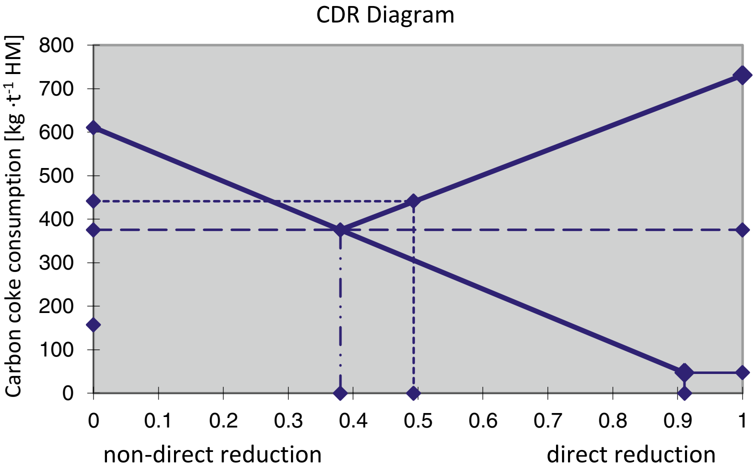


Fig. 8.9 Determination of kinetic and heat limits of carbon consumption (modified CDR diagram)

8.4 Conclusion

The mathematical model of indirect reduction describes well the reduction in the zone of blast furnace where the effect of the Boudouard reaction is insignificant. But this model might be also successfully employed for simulation of the reduction process of the so-called direct reduction iron (DRI) where coke is not a part of the burden. First of all, the degree of the charge metallization reached at the outlet of the charge from the bottom part of such a countercurrent reactor is important for evaluation of the simulation results of these alternative iron production processes. The calculation of concentration profiles using mathematical modeling can be carried out for different specific consumptions of the reduction gas in this countercurrent reactor. The simulation then enables a prediction of the degree of metallization (pre-reduction) for various alternatives of ore charges (ore, pellets, sinters).

A simulation study of the reduction using kinetic model enables us to determine the limits posed by the thermal conditions and the kinetics of the reduction. It also enables more objective assessment of the impact of the considered innovations in the pig iron production.

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References

Babich A, Senk D, Gudenau HW, Mavrommatis KTh (2008) Ironmaking, 1st edn. Wissenschaftsverlag Mainz, Aachen

Bilík J (1990) Matematický model degradace koksu ve vysoké peci. Hutnické listy XLV(4): 225–230

Bilík J, Vu HM (2000) Komplexní kinetický model redukce oxidů železa ve vysoké peci. Hutnické listy 4–7:7–10

Bilík J, Pustějovská P, Jursová S (2013) In: Kledusová J (ed) Modelování, analýza a predikce pochodů výroby železa z hlediska současných energetických a ekologických požadavků, 1st edn. Akademické nakladatelství Cerm, s.r.o. Brno

Jursová S, Bilík J (2013) Innovative research in the field of reductive processes. doi:10.5593/SGEM2013/BA1.V2/S04.008

Jursová S, Pustějovská P, Brožová S, Bilík J (2013) Optimization of blast furnace process according to metallurgical materials reducibility. In: Staniewska E, Górska M (eds) Doskonalenie procesów produkcyjnych i logistycznych, 1st edn. Wydawnictwo Wydziału Inżynierii Procesowej, Materiałowej i Fizyki Stosowanej Politechniki Częstochowskiej. Czestochowa

Jursová S, Pustějovská P, Brožová S, Bilík J (2015) Evaluation of low-reducible sinter in blast furnace technology by mathematical model developed at Centre ENET, VSB – Technical university of Ostrava. Int J Mech Aeros Ind Mechatron Eng 9(4):585–588

Konstanciak A, Jowsa J, Derda W (2003) Computer simulation of change in the chemical composition of coke ash in the blast-furnace. Mater Sci Forum 426–4:4535–4540

Mihok Ĺ, Baricová D (2008) Modern operating and verification methods in ironmaking and steelmaking metallurgy, 1st edn. Elfa, Košice

Pustějovská P, Jursová S (2013a) Effect of waste and alternative fuels on blast-furnace operation. Metallurgist 56(11):908–911

Pustějovská P, Jursová S (2013b) Process engineering in iron production. Chem Process Eng 34(1):63–76

Pustejovska P, Jursova S, Brozova S (2013) Determination of kinetic constants from tests of reducibility and their application for modelling in metallurgy. J Chem Soc Pak 35(3):565–569

Pustějovská P, Tůma J, Staněk V, Křišťál J, Jursová S, Bilík J (2015) Using a mathematical model of counter-current flow in a blast furnace to evaluate reducibility of iron-ore-bearing raw materials. Steel Res Int 86(4):320–328